Scribing-0803_second class

Liuxuan Yu, Mengnan He, Anying Li

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K-means is fast and efficient, be the first try. The second go-to algorithm: hierarchical clustering.

Strength of Hierarchical clustering:

(1) Do not have to decide the number of cluster upfront
(2) Can be very interpretable.

Limitations of Hierarchical clustering:

(1) Computational complexity: O(N3)
(2) Choice of linkage is important

- sensitive to noise/outliers
- difficulty of different sized clusters

(3) Once you decided to break or combine a cluster, you can't undo it.
(4) No objective function is directly minimized

Two categories of Hierarchical clustering:

(1) Divisive: from trunk and then upside down

(2) Agglomerative: from leaf to the whole tree
  – start everything with its own cluster;
  – collection of points and clusters

Key input: linkage criterion

How to split and merge? how to define the distance?

1. Centroid: distance between centers
2. Min/single: distance between the closest points/clusters
3. Max/complete: distance between furthest points or clusters
4. Average: average distance of all possible pairs

- Whether you choose divisive or agglomerative, they both need linkage criterion!

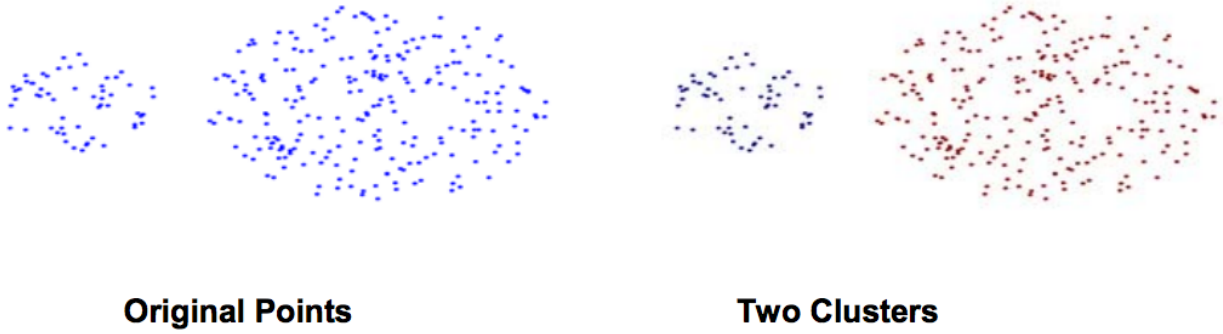


Figure 1:

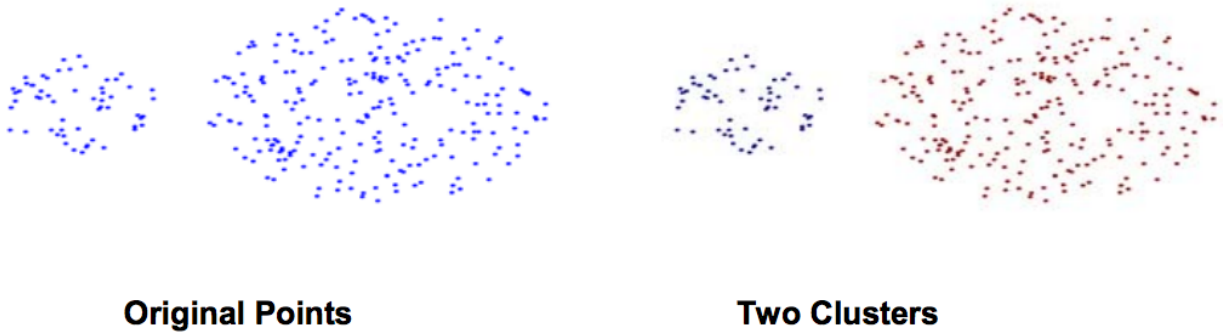


Figure 2: **strength of min/single: can handle non-elliptical shapes**

Figure 3: **weakness of min/single: sensitive to outliers and noise**

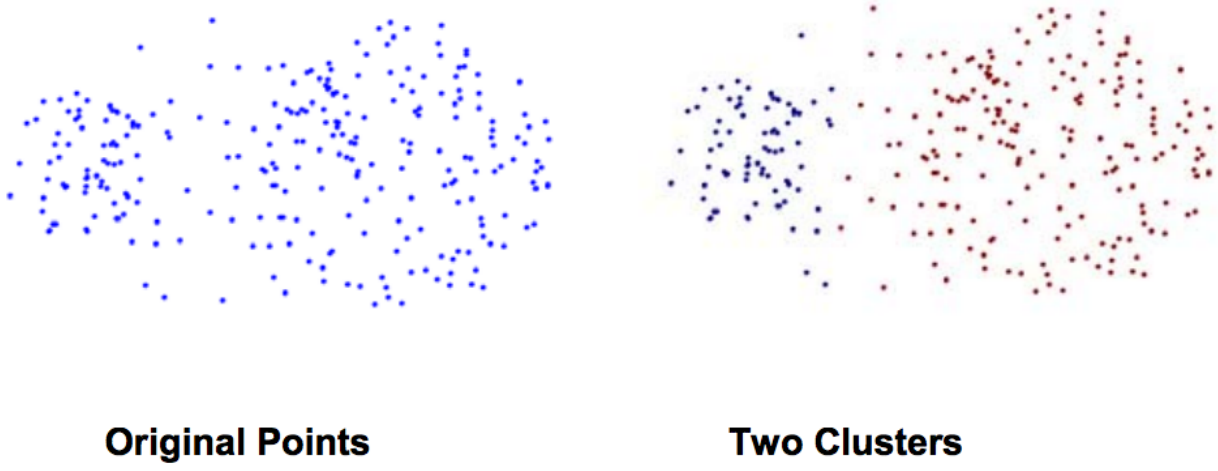


Figure 4: **strength of max/complete: more robust to noise and outliers**

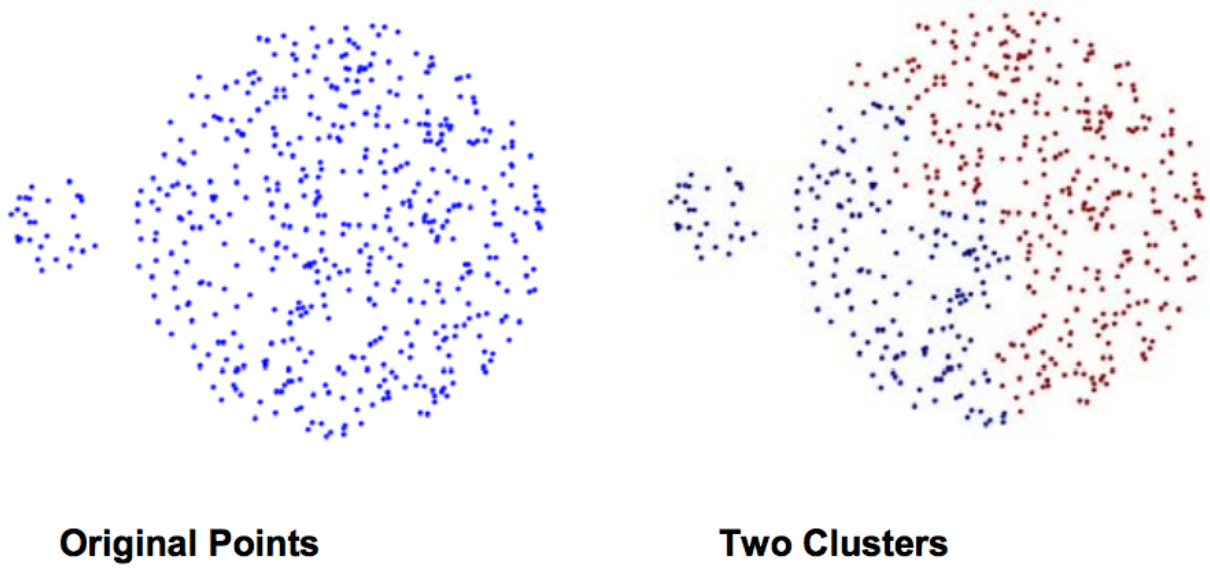


Figure 5: **weakness of max/complete: tend to break large clusters**

Here are some keypoints of the hierarchical clustering R script

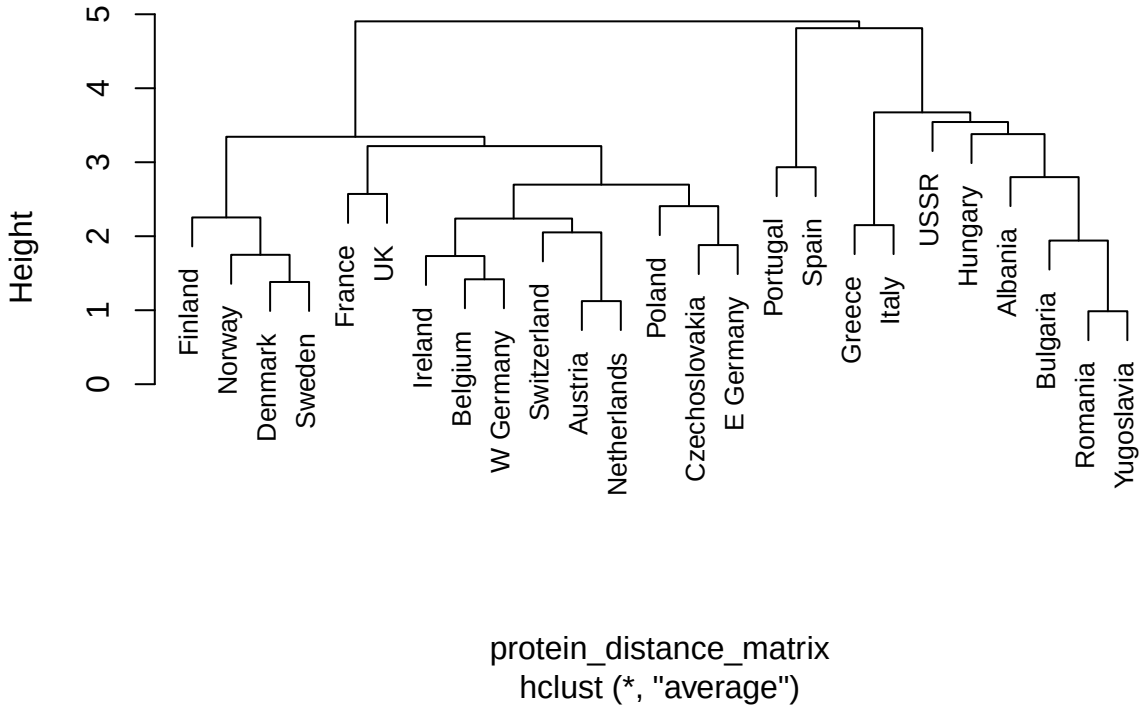
```
protein <- read.csv("protein.csv", row.names=1)
protein_scaled <- scale(protein, center=TRUE, scale=TRUE)
```

1. Form a pairwise distance matrix using the dist function

```
protein_distance_matrix = dist(protein_scaled, method='euclidean')
```

2. Run hierarchical clustering and then cut the tree into 5 clusters.

```
hier_protein = hclust(protein_distance_matrix, method='average')
plot(hier_protein, cex=0.8)
```



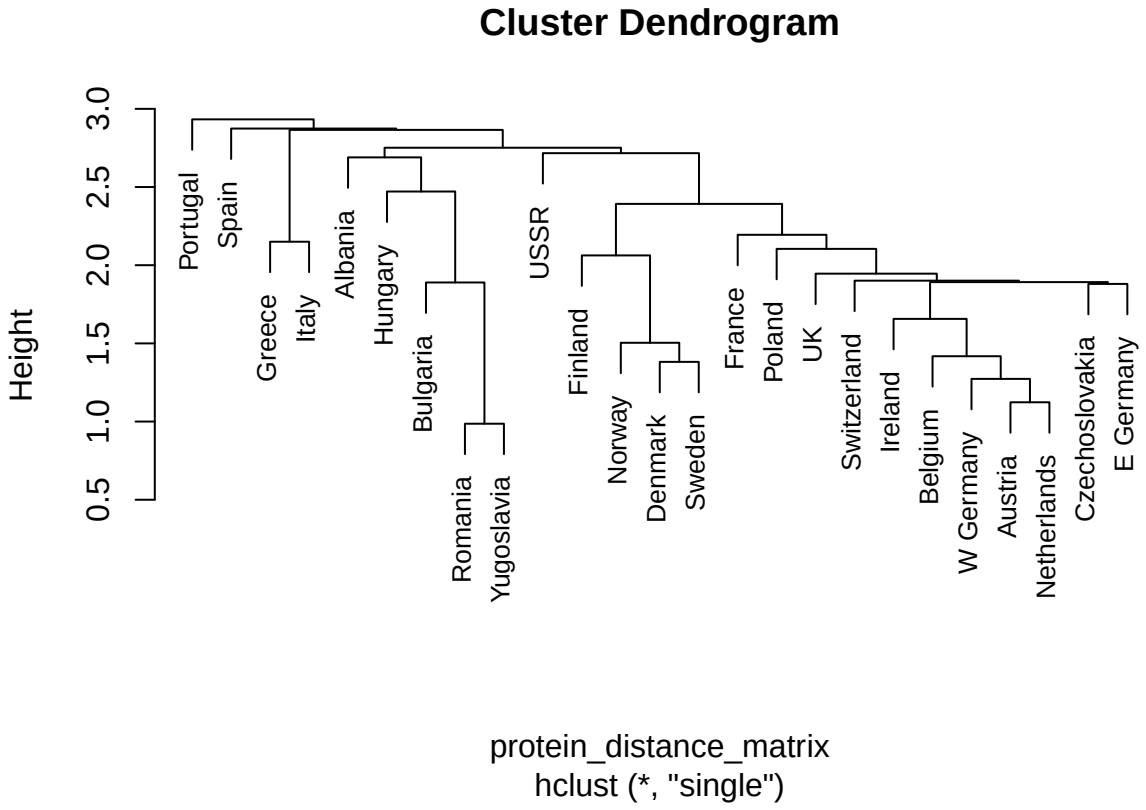

```
cluster1 = cutree(hier_protein, k=5)
```

3. This is to tell which cluster each country is in

```
which(cluster1 == 1)
which(cluster1 == 2)
which(cluster1 == 3)
```

4. Use single linkage instead. The structure of the tree is more unbalanced than the first one.

```
hier_protein2 = hclust(protein_distance_matrix, method='single')
plot(hier_protein2, cex=0.8)
```


Cluster Dendrogram
Height
0.5
1.0
1.5
2.0
2.5
3.0
Portugal
Spain
Greece
Italy
Albania
Hungary
Bulgaria
Romania
Yugoslavia
USSR
Finland
Norway
Denmark
Sweden
France
Poland
UK
Switzerland
Ireland
Belgium
W Germany
Austria
Netherlands
Czechoslovakia
E Germany
protein_distance_matrix
hclust (*, "single")